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Computational framework for the regularised 20-moment equations for non-equilibrium gas flows

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SUMMARY

The paper presents a framework to solve the regularised 20 moment equations consisting of a set of transport-like governing equations, the required constitutive closure, re-casting of the equations in second-order partial derivative form and derivation of additional wall boundary conditions. Couette flow results reveal that good agreement occurs between the 20 moment equations and direct simulation Monte Carlo data.

KEY WORDS: Gas microfluidics ; Non-equilibrium gas flows ; Wall boundary conditions; Method of moments

1. INTRODUCTION

The viable manufacture of miniaturised devices, on the order of microns or sub-microns, has been made possible through recent technological developments. However, these advances have not been matched by an improved fundamental understanding of the rich multiphysics occuring in micro-electro-mechanical systems (MEMS) [1]. In particular, microscale gas flows provide a lot of challenges in terms of predicting correctly and efficiently many of the observed non-equilibrium phenomena.

Non-equilibrium effects occur when the mean free path, λ, is similar to the characteristic length of the flow domain *e.g.* channel height, H. The Knudsen number, $Kn = \lambda/H$, is a dimensionless parameter characterising non-equilibrium effects in gas flows identifiying various regimes [2]. For $0.1 < Kn < 10$, the flow is in the transition regime, and the Navier-Stokes-Fourier (NSF) equations are no longer considered to be valid due to the onset of various non-equilibrium effects. Alternative approaches are needed to model flows in this regime by means of either discrete methods or extended continuum modelling. Discrete methods such as direct

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simulation Monte Carlo (DSMC) provide a stochastic solution to the nonlinear Boltzmann equation but are known to be computationally intensive, especially for the low speed flows typically encountered in MEMS [3].

The method of moments, developed by Grad [4], replaces the Boltzmann equation with a hierarchy of partial differential equations (PDEs) particularly providing closure for 13 equations (G13) where on top of the conservation equations of mass, momentum and energy additional balance laws for viscous stress and heat flux were derived. Torrilhon and Struchtrup [5] and Struchtrup [6, 7] provided a different closure through regularisation of Grad's equations (R13), which provide better resolution of non-equilibrium phenomena and are proven to be stable both in space and time. Gu and Emerson [8] cast the equations in a second-order PDE form and provide Maxwellian type wall boundary conditions (WBCs) [9]. Noticeable improvements over the classical NSF solutions were observed. The present study follows a similar strategy using a regularised 20-moment (R20) equation set which is derived together with the constitutive closure. Subsequently the equations are re-cast in a second-order PDE form and additional WBCs are provided.

2. REGULARISED 20 MOMENT EQUATIONS

The conservation equations for mass, momentum and energy in terms of position, x_i, and time, t, are given by,

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_i}{\partial x_i} = 0, \tag{1}$$

$$\rho\frac{Dv_i}{Dt} + \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} = 0 \quad \text{and} \tag{2}$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \frac{\partial q_i}{\partial x_i} + (p\delta_{ij} + \tau_{ij})\frac{\partial v_i}{\partial x_j} = 0, \tag{3}$$

where δ_{ij} is the Kronecker delta, ρ is the density, v_i is the flow velocity, $p = \rho\theta$ is the pressure and $\theta = RT$ is the specific energy related to the specific gas constant, R, and temperature, T. D/Dt is the material derivative and repeated indices indicate a tensor contraction. Relations for viscous stress, τ_{ij}, and heat flux, q_i, are required in order to close the above 5-moment equation set. The governing equations for τ_{ij} and q_i derived by Grad [4] are written here together with an additional transport equation for m_{ijk}, where for Maxwell molecules,

$$\frac{D\tau_{ij}}{Dt} + \frac{\partial m_{ijk}}{\partial x_k} + \underline{2p\frac{\partial v_{<i}}{\partial x_{j>}}} + \frac{4}{5}\frac{\partial q_{<i}}{\partial x_{j>}} + \tau_{ij}\frac{\partial v_k}{\partial x_k} + 2\tau_{k<i}\frac{\partial v_{j>}}{\partial x_k} = -\frac{p\tau_{ij}}{\mu}, \tag{4}$$

$$\begin{aligned}&\frac{Dq_i}{Dt} + \underline{\underline{\frac{1}{2}\frac{\partial R_{ij}}{\partial x_j}}} + \underline{\underline{\frac{1}{6}\frac{\partial \Delta}{\partial x_i}}} + m_{ijk}\frac{\partial v_j}{\partial x_k} + \underline{\frac{5p}{2}\frac{\partial \theta}{\partial x_i}} + \theta\frac{\partial \tau_{ij}}{\partial x_j} + \frac{7}{2}\tau_{ij}\frac{\partial \theta}{\partial x_j} - \frac{\tau_{ij}}{\rho}\frac{\partial p}{\partial x_j} - \frac{\tau_{ij}}{\rho}\frac{\partial \tau_{jk}}{\partial x_k} + \\ &\frac{7}{5}q_i\frac{\partial v_j}{\partial x_j} + \frac{7}{5}q_j\frac{\partial v_i}{\partial x_j} + \frac{2}{5}q_j\frac{\partial v_j}{\partial x_i} = -\frac{2pq_i}{3\mu} \quad \text{and}\end{aligned} \tag{5}$$

$$\begin{aligned}&\frac{Dm_{ijk}}{Dt} + \underline{\underline{\frac{\partial \phi_{ijkl}}{\partial x_l}}} + \underline{\underline{\frac{3}{7}\frac{\partial R_{<ij}}{\partial x_{k>}}}} + 3\theta\frac{\partial \tau_{<ij}}{\partial x_{k>}} - \frac{3\tau_{<ij}}{\rho}\left(\theta\frac{\partial \rho}{\partial x_{k>}} + \frac{\partial \tau_{k>l}}{\partial x_l}\right) + m_{ijk}\frac{\partial v_l}{\partial x_l} + \\ &3m_{l<ij}\frac{\partial v_{k>}}{\partial x_l} + \frac{12}{5}q_{<i}\frac{\partial v_j}{\partial x_{k>}} = -\frac{3pm_{ijk}}{2\mu},\end{aligned} \tag{6}$$

where R_{ij}, Δ, m_{ijk} and ϕ_{ijkl} are higher-order moments and the angular brackets $<>$ represent the traceless part of a tensor. Regularisation for the first five moments yields the NSF equations, as indicated by the single underlined terms in Equations (4) and (5). A similar regularisation procedure on a 13-moment set would yield constitutive expressions similar to those derived by Torrilhon and Struchtrup [5] where

$$m_{ijk}{}^{R13} = -\frac{2\mu}{p}\left(\theta\frac{\partial\tau_{<ij}}{\partial x_{k>}} - \frac{\tau_{<ij}}{\rho}\left(\theta\frac{\partial\rho}{\partial x_{k>}} + \frac{\partial\tau_{k>l}}{\partial x_l}\right) + \frac{4}{5}q_{<i}\frac{\partial v_j}{\partial x_{k>}}\right), \tag{7}$$

$$\begin{aligned} R_{ij}{}^{R13} = -\frac{6\mu}{7p}\Bigg(&\frac{28}{5}\theta\frac{\partial q_{<i}}{\partial x_{j>}} - \frac{8\tau_{ij}\theta}{3}\frac{\partial v_k}{\partial x_k} + \frac{56}{5}q_{<i}\frac{\partial\theta}{\partial x_{j>}} - \frac{28q_{<i}}{5\rho}\frac{\partial p}{\partial x_{j>}} + 4\theta\tau_{k<i}\frac{\partial v_{j>}}{\partial x_k} + \\ &4\theta\tau_{k<i}\frac{\partial v_k}{\partial x_{j>}} - \frac{14\tau_{ij}}{3\rho}\frac{\partial q_k}{\partial x_k} - \frac{14\tau_{ij}\tau_{kl}}{3\rho}\frac{\partial v_k}{\partial x_l} - \frac{28q_{<i}}{5\rho}\frac{\partial\tau_{j>k}}{\partial x_k} + \frac{2p}{3\mu\rho}\tau_{k<i}\tau_{j>k}\Bigg) \quad \text{and} \end{aligned} \tag{8}$$

$$\Delta^{R13} = -\frac{3\mu}{2p}\left(8\theta\tau_{ij}\frac{\partial v_i}{\partial x_j} - \frac{8q_i}{\rho}\frac{\partial p}{\partial x_i} - \frac{8q_i}{\rho}\frac{\partial\tau_{ij}}{\partial x_j} + 8\theta\frac{\partial q_i}{\partial x_i} + 28q_i\frac{\partial\theta}{\partial x_i} + \frac{2p\tau_{ij}\tau_{ij}}{3\mu\rho}\right). \tag{9}$$

From Equations (4 – 6), it can be shown that a closure relationship is required for R_{ij}, Δ and ϕ_{ijkl}, indicated by the double-underlined terms. Equations (8) and (9) are used to provide closure relationships for R_{ij} and Δ, whereas m_{ijk} will be solved in its full transport form requiring a closure for ϕ_{ijkl}. Using a generic moment framework, regularisation [7] and a production term for Maxwell molecules [10], it can be shown that

$$\begin{aligned}\phi_{ijkl} = \frac{2400\mu}{5033p}\Bigg(&-4\theta\frac{\partial m_{<ijk}}{\partial x_{l>}} + \frac{4\theta}{\rho}m_{<ijk}\frac{\partial\rho}{\partial x_{l>}} + \frac{4}{\rho}m_{<ijk}\frac{\partial\tau_{l>m}}{\partial x_m} - 12\theta\tau_{<ij}\frac{\partial v_k}{\partial x_{l>}} - \\ &\frac{233p}{800\mu\rho}\tau_{<ij}\tau_{kl>}\Bigg).\end{aligned} \tag{10}$$

In the present paper, Equation (10) is used to close Equation (6).

3. NUMERICAL PROCEDURE

Equations (1 – 5) can be re-cast in conservative form to yield similar expressions to those proposed by Gu and Emerson [8]. Using a similar procedure, Equation (6) is re-cast in conservative form where the convective, diffusive and source terms are identified by solving m_{ijk} as a specific deviation from $m_{ijk}{}^{R13}$, where $\rho c_{ijk} = m_{ijk} - m_{ijk}{}^{R13}$. After some algebraic manipulation, with recursive use of tensor identities and substituting Equations (7) and $m_{ijk} = \rho c_{ijk} + m_{ijk}{}^{R13}$ in Equations (6) and (10), it can be shown that

$$\begin{aligned}&\underbrace{\frac{\partial\rho c_{ijk}v_l}{\partial x_l}}_{\text{convective term}} - \underbrace{\frac{\partial}{\partial x_l}\left(\frac{2400\mu}{5033}\frac{\partial c_{ijk}}{\partial x_l}\right)}_{\text{diffusive term}} = \\ &\underbrace{-\frac{3p\rho c_{ijk}}{2\mu} - \frac{\partial}{\partial x_l}\left(m_{ijk}{}^{R13}v_l\right) - \frac{\partial E_{ijkl}}{\partial x_l} - \frac{3}{7}\frac{\partial R_{<ij}{}^{R13}}{\partial x_{k>}} - 3m_{l<ij}\frac{\partial v_{k>}}{\partial x_l}}_{\text{source term}},\end{aligned} \tag{11}$$

where

$$E_{ijkl} = \frac{2400\mu}{5033p}\left(-\theta c_{ijk}\frac{\partial \rho}{\partial x_l} - \theta\frac{\partial m_{ijk}{}^{R13}}{\partial x_l} - \theta\frac{\partial m_{ijl}}{\partial x_k} - \theta\frac{\partial m_{ikl}}{\partial x_j} - \theta\frac{\partial m_{jkl}}{\partial x_i} + \frac{4\theta}{\rho}m_{<ijk}\frac{\partial \rho}{\partial x_{l>}} + \frac{4}{\rho}m_{<ijk}\frac{\partial \tau_{l>m}}{\partial x_m} + \frac{24}{7}\theta\delta_{(ij}\left.\frac{\partial m_{kl)m}}{\partial x_m}\right|_s - 12\theta\tau_{<ij}\frac{\partial v_k}{\partial x_{l>}} - \frac{233p}{800\mu\rho}\tau_{<ij}\tau_{kl>}\right). \tag{12}$$

Round brackets around subscripts $(ijkl)$ in Equation (12) indicate symmetrised tensors and the subscript, s, indicates symmetrised gradients. In this form, additional WBCs for c_{ijk} are required through arguments on m_{ijk}.

4. MAXWELLIAN WALL BOUNDARY CONDITIONS FOR m_{ijk}

Wall boundary conditions for v_i, T, τ_{ij} and q_i, suitable for a 13-moment set, were derived by Gu and Emerson [8] using a Grad 35 moment distribution function and a Maxwellian scattering kernel at the wall. The Maxwellian kernel is applicable to odd moments with respect to the normal velocity to the wall, C_2, so that the half flux integrals remain valid in the limit of a vanishing accommodation coefficient, α [4]. Thus the additional moments considered for a 20 moment case in two dimensions are $\psi = \left(C^2C_1C_1C_1C_2, C_1C_1C_2C_2C_2, C_1C_1C_1C_2C_2C_2, C_2C_2C_2C_2C_2\right)$, where C_1 is the peculiar velocity of molecules parallel to the wall. This moment set will yield the new additional WBCs,

$$m_{111} = \pm\frac{2-\alpha}{\alpha}\sqrt{\frac{\pi}{2\theta}}\left(\frac{11\phi_{1112}+27\theta\tau_{12}}{10} + \frac{27R_{12}}{35}\right) - \frac{12q_1}{5} - \frac{3m_{122}}{2} - \frac{\rho_w}{10}\sqrt{\frac{v_{1s}{}^5}{\theta^3}}\left(24\theta_w{}^2 + 13\theta_w v_{1s}^2 + v_{1s}^4\right), \tag{13}$$

$$m_{112} = \pm\frac{\alpha}{2-\alpha}\sqrt{\frac{1}{2\pi\theta}}\left(2\phi_{1122} + 2\theta\tau_{22} + \frac{4\theta\tau_{11}}{3} + \frac{\phi_{2222}}{6} + \frac{\Delta}{6} + \frac{3R_{22}}{7} + \frac{2R_{11}}{7} + \frac{4\rho\theta^2}{3} - \frac{4}{3}\sqrt{\frac{\theta_w}{\theta}}\rho_w\theta_w\left(v_{1s}^2+\theta_w\right)\right) - \frac{4q_2}{5} - \frac{m_{222}}{3}, \tag{14}$$

$$m_{122} = \pm\frac{2-\alpha}{\alpha}\sqrt{\frac{\pi}{2\theta}}\left(\frac{\phi_{1112}}{3} + \frac{\phi_{1222}}{3} + \frac{2R_{12}}{7} + \theta\tau_{12}\right) - \frac{2}{3}\left(v_{1s}\rho_w\left(\frac{\theta_w}{\theta}\right)^{\frac{3}{2}}\left(\frac{v_{1s}{}^2}{3}+\theta_w\right) + q_1 + \frac{m_{111}}{3}\right) \quad \text{and} \tag{15}$$

$$m_{222} = \pm\frac{\alpha}{2-\alpha}\frac{1}{\sqrt{2\pi\theta}}\left(4\theta\tau_{22} + \phi_{2222} + \frac{\Delta}{5} + \frac{6R_{22}}{7} + \frac{8\left(\rho\theta^2\sqrt{\theta} - \rho_w\theta_w^2\sqrt{\theta_w}\right)}{5\sqrt{\theta}}\right) - \frac{6q_2}{5}, \tag{16}$$

where

$$\rho_w = \frac{1}{\sqrt{\theta\theta_w}}\left(p + \frac{\tau_{22}}{2} - \frac{35\phi_{2222}+7\Delta+30R_{22}}{840\theta}\right), \tag{17}$$

and v_{1s} is the slip velocity and $\theta_w = RT_w$ is the wall specific energy.

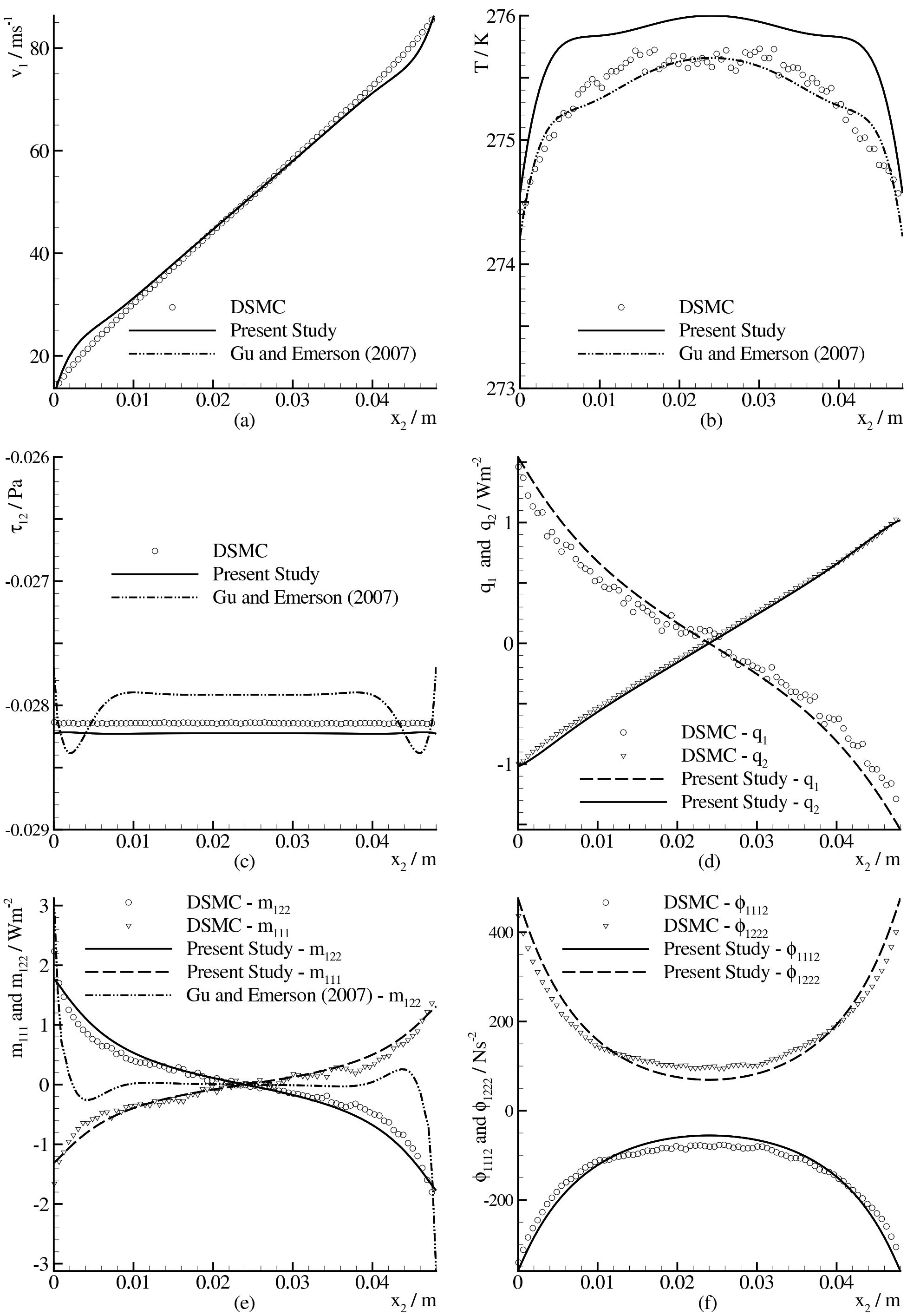

Figure 1. Couette flow results for $Kn = 0.25$; Profiles for (a) tangential velocity, (b) temperature, (c) shear stress, (d) heat fluxes, (e) m_{111}, m_{122} and (f) ϕ_{1112}, ϕ_{1222}.

5. RESULTS

Figure 1 compares Couette flow results for the proposed R20 equations against DSMC data and the results by Gu and Emerson [8] for $Kn = 0.25$ and a Mach number of 0.32. Argon was used as a model gas for a plate seperation of 0.048 m at a total pressure of 0.532 Pa with the wall temperatures set at $T_w = 273$ K. No empirical corrections were imposed on the WBCs both on those derived by Gu and Emerson [8] and the additional conditions derived in this study.

6. DISCUSSION AND CONCLUSIONS

From Figures 1 (a), (c) and (e) it can be seen that the spurious behaviour close to the wall boundary, reported for the R13 equations [8], is significantly attenuated when using an R20 formulation. Non-equilibrium effects are most siginificant in the Knudsen layer, a kinetic boundary layer occuring in close proximity to solid walls. This might indicate that larger moment sets improve the physical description of rarefied gas flows by making use of an extended approximation of the distribution function. The additional equations solved in combination with the newly derived boundary conditions are strongly coupled with the stress equation and contribute better to the diffusive process for stress, hence improving the agreement with DSMC. However, from Figure 1 (b), it is evident that the temperature profile is not so well resolved since an R13 closure is used for the heat flux equation, even though the temperature variation is minimal. Resolving these closure terms in their full transport form, by making use of a regularised 26 moment equation set, should improve the prediction of the temperature profile.

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